



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 03:58 PM EDT

PDB ID : 1I97 / pdb_00001i97
Title : CRYSTAL STRUCTURE OF THE 30S RIBOSOMAL SUBUNIT FROM THERMUS THERMOPHILUS IN COMPLEX WITH TETRACYCLINE
Authors : Pioletti, M.; Schlutzen, F.; Harms, J.; Zarivach, R.; Gluehmann, M.; Avila, H.; Bartels, H.; Jacobi, C.; Hartsch, T.; Yonath, A.; Franceschi, F.
Deposited on : 2001-03-18
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

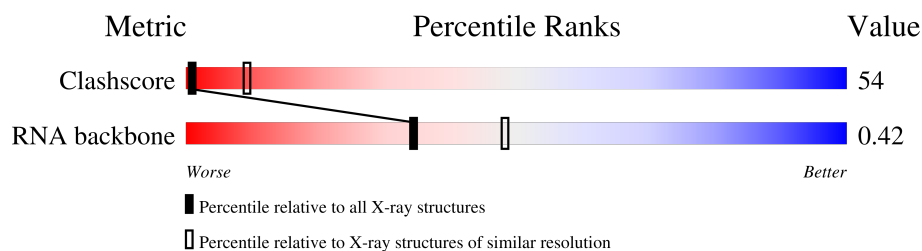
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

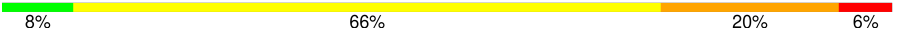
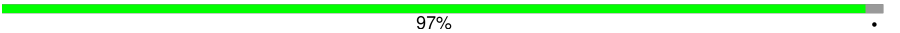
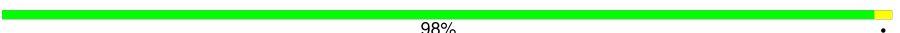
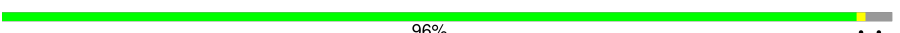
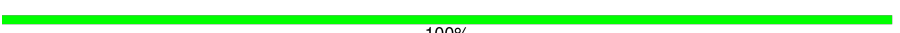
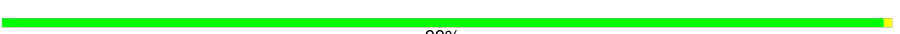
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1002 (5.06-3.94)
RNA backbone	3983	1039 (5.90-3.10)

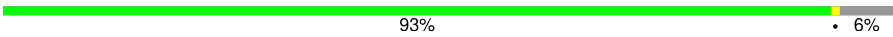
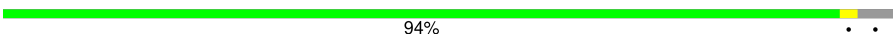
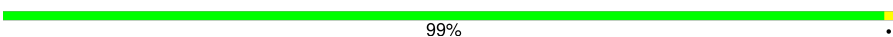
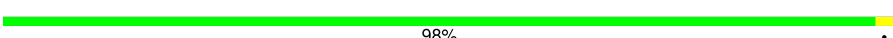
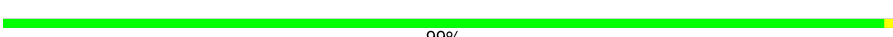
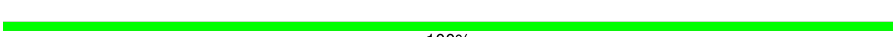
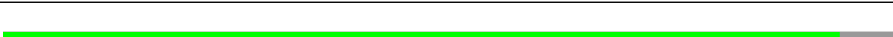
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1514	 8% 66% 20% 6%
2	B	255	 97% .
3	C	238	 87% 13%
4	D	208	 98% .
5	E	161	 96% ..
6	F	101	 100%
7	G	155	 99% .
8	H	138	 100%
9	I	128	 97% ..

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Mol	Chain	Length	Quality of chain
10	J	104	 93% 6%
11	K	128	 94% . .
12	L	131	 99% .
13	M	125	 74% . 26%
14	N	60	 98% .
15	O	88	 99% .
16	P	88	 100%
17	Q	104	 99% .
18	R	87	 94% 6%
19	S	92	 87% 13%
20	T	105	 94% 6%
21	U	26	 88% . 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	TAC	A	2001	X	-	X	-
24	TAC	A	2003	X	-	X	-
24	TAC	A	2004	X	-	X	-
24	TAC	A	2005	X	-	X	-
24	TAC	A	2006	X	-	X	-
24	TAC	D	2002	X	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 36361 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0	0
			32534	14482	6022	10517	1513			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	249	Total	C	0	0	249
			249	249			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	206	Total	C	0	0	206
			206	206			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	208	Total	C	0	0	208
			208	208			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	E	156	Total	C	0	0	156
			156	156			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	F	101	Total	C	0	0	101
			101	101			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	155	Total C 155 155	0	0	155

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	138	Total C 138 138	0	0	138

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	127	Total C 127 127	0	0	127

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	98	Total C 98 98	0	0	98

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	123	Total C 123 123	0	0	123

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	131	Total C 131 131	0	0	131

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	M	93	Total C 93 93	0	0	93

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	N	60	Total C 60 60	0	0	60

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	O	88	Total C 88 88	0	0	88

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	P	88	Total C 88 88	0	0	88

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	Q	104	Total C 104 104	0	0	104

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	R	82	Total C 82 82	0	0	82

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	S	80	Total C 80 80	0	0	80

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	T	99	Total C 99 99	0	0	99

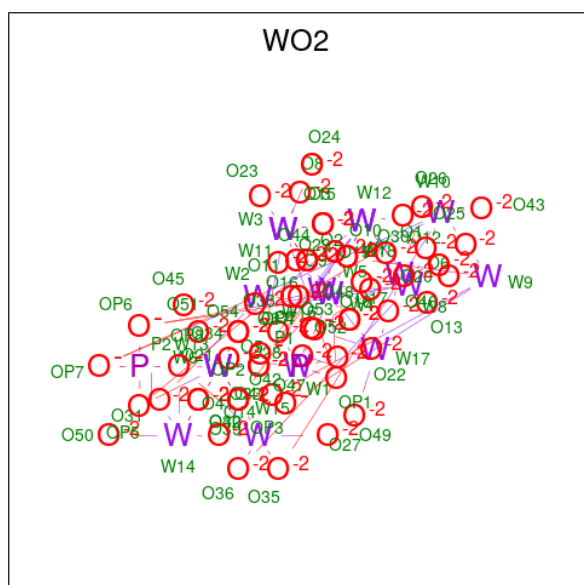
- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	U	24	Total C 24 24	0	0	24

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	63	Total 63 Mg 63	0	0
22	D	2	Total 2 Mg 2	0	0
22	E	1	Total 1 Mg 1	0	0
22	G	1	Total 1 Mg 1	0	0
22	K	1	Total 1 Mg 1	0	0
22	L	1	Total 1 Mg 1	0	0
22	P	1	Total 1 Mg 1	0	0
22	Q	2	Total 2 Mg 2	0	0
22	T	3	Total 3 Mg 3	0	0

- Molecule 23 is OCTADECATUNGSTENYL DIPHOSPHATE (CCD ID: WO2) (formula: $\text{O}_{62}\text{P}_2\text{W}_{18}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total 82	O 62	P 2	W 18	0	0
23	A	1	Total 82	O 62	P 2	W 18	0	0
23	A	1	Total 82	O 62	P 2	W 18	0	0
23	A	1	Total 82	O 62	P 2	W 18	0	0
23	B	1	Total 82	O 62	P 2	W 18	0	0
23	B	1	Total 82	O 62	P 2	W 18	0	0
23	B	1	Total 82	O 62	P 2	W 18	0	0
23	D	1	Total 82	O 62	P 2	W 18	0	0
23	E	1	Total 82	O 62	P 2	W 18	0	0
23	G	1	Total 82	O 62	P 2	W 18	0	0
23	H	1	Total 82	O 62	P 2	W 18	0	0
23	J	1	Total 82	O 62	P 2	W 18	0	0
23	K	1	Total 82	O 62	P 2	W 18	0	0
23	R	1	Total 82	O 62	P 2	W 18	0	0

- Molecule 24 is TETRACYCLINE (CCD ID: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	A	1	Total 32	C 22	N 2	O 8	0	0
24	D	1	Total 32	C 22	N 2	O 8	0	0

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

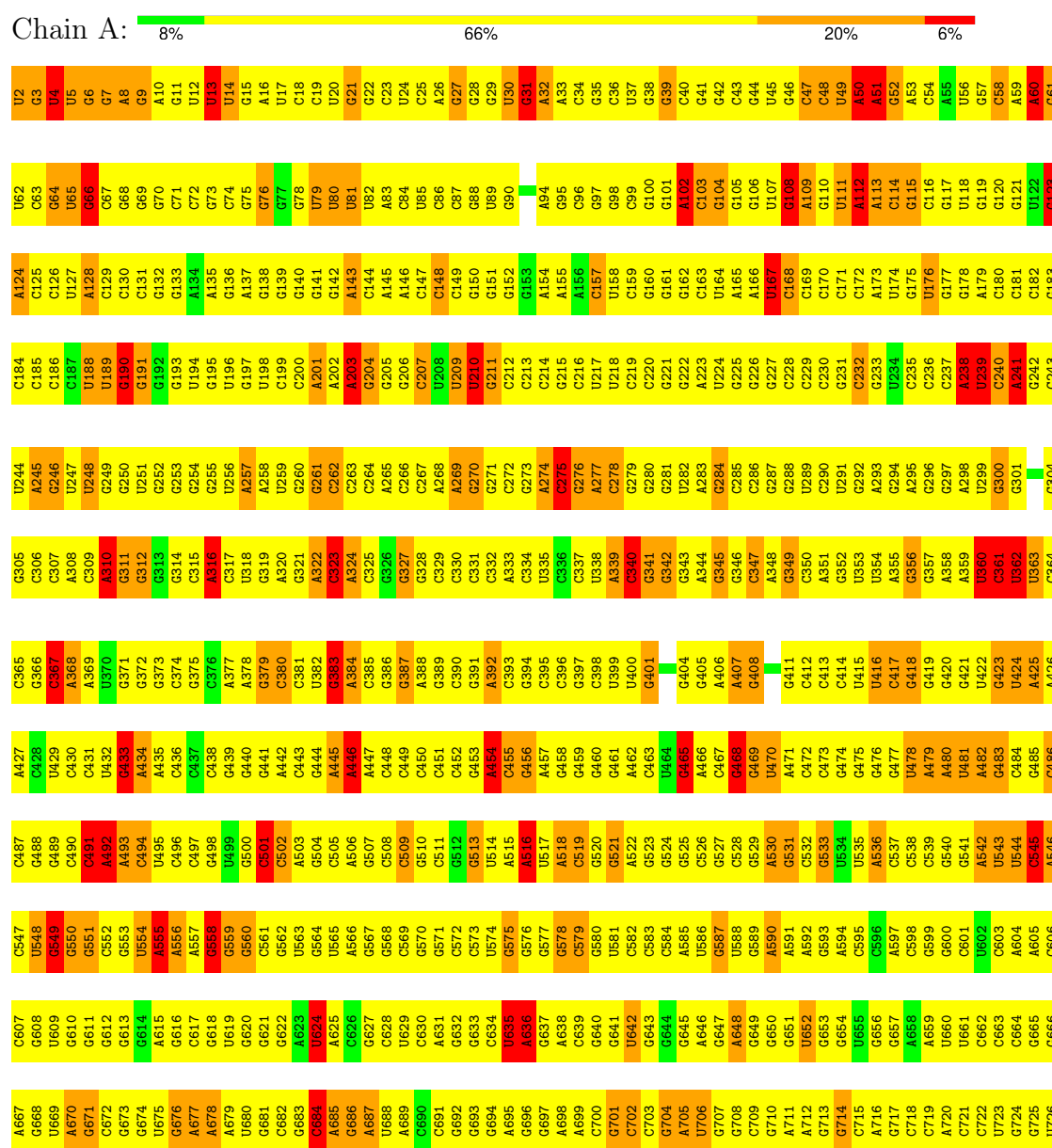
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	D	1	Total Zn 1 1	0	0
25	N	1	Total Zn 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

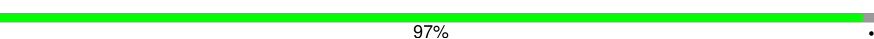
Note EDS was not executed.

• Molecule 1: 16S RRNA



A1470	C1278	U968	G1032	A1092	G1154	U1216	C1278	A1338	G1400	A1470
G1471	C728	C909	C1033	A1093	G1155	A1217	C1279	U1339	G1401	G1471
A1472	C729	G910	U1034	C1094	G1156	A1218	A1280	C1340	C1402	A1472
C1473	C730	C911	G1035	C1095		A1219	A1281	A1341		C1473
G1474	C731	A912	C1036	C1096	G1159	U1220	U1282	C1342	C1406	G1474
U1475	C732	C913	A1037	C1097	G1160	U1221	U1283	C1343	U1407	U1475
A1476	C733	A914	U1038	C1098	A1161	G1222	C1284	C1344	C1408	A1476
A1477	G734	A915	G1039	G1099	G1162	C1223	C1285	U1345	U1409	A1477
C1478	U735	A916	C1040	C1100	G1163	C1224	G1286	A1346	A1410	C1478
A1479	U736	C917	C1041	C1101	G1164	C1225	U1287	C1347	A1411	A1479
G1481	C737	G918	C1042	A978	G1165	A1226	U1288	C1348	C1412	A1480
G1482	C738	C919	C1043	G979	G1166	C1227	U1289	C1349	G1413	G1481
U1483	C739	U920	U1044	G980	G1167	U1228	G1290	G1350	G1414	G1482
A1484	C800	C921	C1045	G981	G1168	A1229	G1291	C1351	A1415	U1483
G1485	C801	G922	G1046	A982	A1169	C1230	G1292	G1352	G1416	A1484
A1486	C802	A923	U1047	A983	C1170	A1231	G1293	G1353	G1417	G1485
G1487	C803	G924	C1048	C984	G1171	A1232	U1294	U1354		A1486
U1488	C804	C925	U1049		A1172	A1233	C1295	G1355	C1421	G1487
U1489	C805	G926	A1050		C1173	U1234	U1296	A1356	C1422	U1488
A1490	C806	U927	C1051	G988	G1174	C1235	G1297	A1357	G1423	U1489
C1491	C807	U928	C1052	U990	U1175	G1236	C1298	U1358	U1424	A1490
C1492	C808	U929	G1053	G991	C1176	A1237	A1299	C1359	G1425	C1491
G1493	C809	G930	C1054	A992	U1177	U1238	A1300	C1360	A1426	G1492
A1494	C810	G931	U1055	A993	G1178	C1301	C1302	G1361	G1427	G1493
A1495	C811	U932	C1056	A994	G1179	C1240	G1303	U1362	C1428	G1494
A1496	C812	U933	C1057	G995	U1180	C1241	G1304	U1363	C1429	A1495
G1497	C813	U934	G1058	C996	U1181	A1242	G1305	C1364	U1430	A1496
U1498	C814	A935	C1059	C997	A1182	C1243	A1306	C1365	A1431	G1497
U1499	C815	G936	U1060	U998	G1183	C1244	C1307	C1366	C1432	U1498
G1500	C816	A937	G1061	G999	C1184	C1245	C1308	G1367	A1433	U1499
C1501	C817	U938	C1062	G1000	G1185	G1246	C1309	G1368	G1434	G1500
A1502	C818	C939	G1063	G1001	U1186	G1247	A1310	C1369	G1435	C1501
G1503	C819	G940	C1064	G1002	G1187	C1248	G1311	C1370	C1436	A1502
C1504	C820	A941	U1065	U1003	G1188	A1249	G1312	C1371	A1437	G1503
U1505	C821	U882	C1066	G1004	C1189	C1250	A1313	U1372	G1438	C1504
G1506	C822	C881	U1067	C1005	C1190	C1251	A1314	G1373	G1439	U1505
A1507	C823	U824	C1068	G1006		C1252	G1315	U1374	C1440	G1506
U1508	C824	A884	U1069		U1193	G1253	C1316	U1375		A1507
U1509	C825	A885	G1070	C1010	A1194		C1317	A1376	C1443	U1508
C1510	C826	A886	G1071	G1011	C1195	G1257	C1318	C1377	G1444	U1509
A1511	C827	C887	U1072	A1012	G1196	C1258	G1319	A1378	A1445	C1510
G1512	C828	U888	U1073	G1013	G1197	U1259	C1320	C1379	A1446	A1511
U1513	C829	C889	A1074	G1014	C1198	A1260	A1321	A1380	G1447	G1512
C1514	C830	A890	C1075	G1015	C1199	A1261	U1322	C1381	C1448	C1513
A1515	C831	A891	G1076	G1016	U1200	U1262	C1323	C1382		U1514
	C832	A892	U1077	A1017	A1139	G1263	G1324	C1383	G1453	G1515
	C833	G953	C1078	G1018	C1140	C1264	C1325	C1384	C1454	
	C834	A954	C1079	G1019	U1141	C1265	U1326	C1385	C1455	
	C835	A955	C1080	G1020	G1142	C1266	A1267	C1386	C1456	
	A836	C956	G1081	C1021	C1143	U1267	G1327	G1387		
	C837	U897	C1082	U1022	C1144	A1268	G1328	U1388	G1459	
	C838	U898	A1023	A1023	C1145	A1269	U1329	U1389		
	C839	G899	G1024	A960	G1146	A1270	A1330	C1391	U1462	
	U840	A900	C1025	G961	C1147	G1271	A1331	G1392	G1463	
	C901	A841	A1026	G962	C1148	U1272	C1332		G1464	
	C842	A842	G963	A963	C1149	U1273	U1333	A1395	G1465	
	C843	G903	A1028	G964	C1150	G1274	G1334	U1396	G1466	
	C904	G904	G1029	G1029	A1151	G1275	C1335	G1397	C1467	
	G905	G905	G1030	G1030	G1152	G1276	G1336	G1398	G1468	
	C967	C967	U1031	U1031	C1215	C1277	G1337	G1399	A1469	

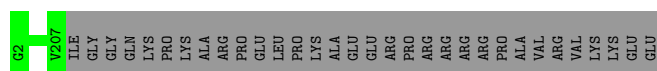
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:  97%



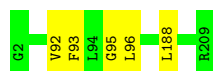
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:  87%



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D: 98% .



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E: 96% ..



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G: 99% .



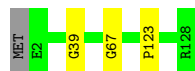
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H: 100%

There are no outlier residues recorded for this chain.

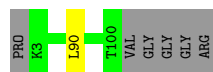
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I: 97% ..



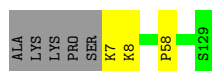
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J: 93% . 6%

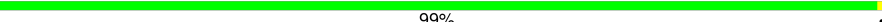


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:  94% . .



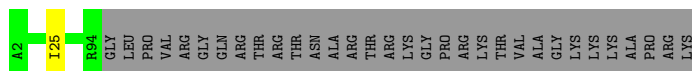
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:  99% .

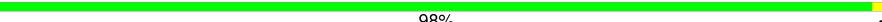


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:  74% . 26%

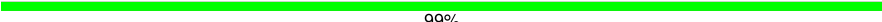


- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain N:  98% .

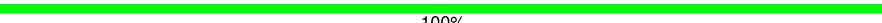


- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:  99% .

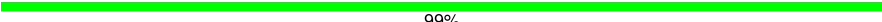


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:  99% .



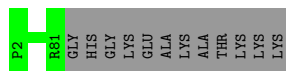
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:  94% 6%



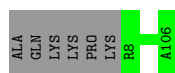
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:
87% 13%



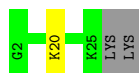
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:
94% 6%



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:
88% 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	406.90 Å 406.90 Å 175.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 4.50	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-4.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36361	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, WO2, TAC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	3/36417 (0.0%)	0.96	144/56838 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	69

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	U	O3'-P	13.93	1.82	1.61
1	A	1178	G	O3'-P	8.48	1.73	1.61
1	A	872	G	O3'-P	6.95	1.71	1.61

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	U	P-O3'-C3'	39.22	179.03	120.20
1	A	871	G	P-O3'-C3'	-36.17	65.94	120.20
1	A	919	G	P-O3'-C3'	34.65	172.17	120.20
1	A	872	G	P-O3'-C3'	-21.89	87.36	120.20
1	A	820	G	P-O3'-C3'	-21.59	87.81	120.20

There are no chirality outliers.

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	U	Sidechain
1	A	21	G	Sidechain
1	A	27	G	Sidechain
1	A	4	U	Sidechain
1	A	50	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32534	0	16424	2777	0
2	B	249	0	0	1	0
3	C	206	0	0	0	0
4	D	208	0	0	12	0
5	E	156	0	0	2	0
6	F	101	0	0	0	0
7	G	155	0	0	2	0
8	H	138	0	0	0	0
9	I	127	0	0	5	0
10	J	98	0	0	1	0
11	K	123	0	0	5	0
12	L	131	0	0	1	0
13	M	93	0	0	1	0
14	N	60	0	0	1	0
15	O	88	0	0	1	0
16	P	88	0	0	0	0
17	Q	104	0	0	3	0
18	R	82	0	0	0	0
19	S	80	0	0	0	0
20	T	99	0	0	0	0
21	U	24	0	0	1	0
22	A	63	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	G	1	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	P	1	0	0	0	0
22	Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	3	0	0	0	0
23	A	328	0	0	0	0
23	B	246	0	0	1	0
23	D	82	0	0	0	0
23	E	82	0	0	1	0
23	G	82	0	0	3	0
23	H	82	0	0	0	0
23	J	82	0	0	1	0
23	K	82	0	0	4	0
23	R	82	0	0	0	0
24	A	160	0	115	159	0
24	D	32	0	23	12	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
All	All	36361	0	16562	2806	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

The worst 5 of 2806 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:U:H1'	24:A:2005:TAC:C9	1.30	1.54
1:A:872:G:C5	1:A:873:C:C5	2.02	1.46
4:D:92:VAL:CA	24:D:2002:TAC:H423	1.41	1.46
1:A:872:G:C5	1:A:873:C:C6	2.11	1.38
1:A:239:U:H1'	24:A:2005:TAC:C8	1.52	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1514 (99%)	323 (21%)	119 (7%)

5 of 323 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	G
1	A	4	U
1	A	5	U
1	A	6	G
1	A	8	A

5 of 119 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	635	U
1	A	1346	U
1	A	866	A
1	A	1345	A
1	A	1514	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 97 ligands modelled in this entry, 77 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	WO2	A	1582	-	54,116,116	64.82	8 (14%)	4,348,348	2.24	1 (25%)
23	WO2	A	1579	-	54,116,116	64.83	8 (14%)	4,348,348	2.23	1 (25%)
24	TAC	A	2001	22	34,35,35	1.95	8 (23%)	43,58,58	2.06	8 (18%)
24	TAC	D	2002	-	34,35,35	1.95	8 (23%)	43,58,58	2.08	8 (18%)
23	WO2	K	1014	-	54,116,116	64.83	8 (14%)	4,348,348	2.23	1 (25%)
24	TAC	A	2004	-	34,35,35	1.96	8 (23%)	43,58,58	2.07	8 (18%)
23	WO2	D	1012	-	54,116,116	64.82	8 (14%)	4,348,348	2.25	1 (25%)
23	WO2	G	1006	-	54,116,116	64.83	8 (14%)	4,348,348	2.23	1 (25%)
23	WO2	A	1581	-	54,116,116	64.83	8 (14%)	4,348,348	2.24	1 (25%)
23	WO2	H	1010	-	54,116,116	64.83	8 (14%)	4,348,348	2.22	1 (25%)
23	WO2	B	1001	-	54,116,116	64.83	8 (14%)	4,348,348	2.24	1 (25%)
23	WO2	A	1580	-	54,116,116	64.83	8 (14%)	4,348,348	2.24	1 (25%)
23	WO2	E	1005	-	54,116,116	64.80	8 (14%)	4,348,348	2.29	1 (25%)
23	WO2	B	1004	-	54,116,116	64.81	8 (14%)	4,348,348	2.26	1 (25%)
24	TAC	A	2005	-	34,35,35	1.94	8 (23%)	43,58,58	2.07	8 (18%)
23	WO2	J	1009	-	54,116,116	64.82	8 (14%)	4,348,348	2.25	1 (25%)
23	WO2	R	1008	-	54,116,116	64.83	8 (14%)	4,348,348	2.23	1 (25%)
24	TAC	A	2003	-	34,35,35	1.96	8 (23%)	43,58,58	2.08	8 (18%)
24	TAC	A	2006	-	34,35,35	1.95	8 (23%)	43,58,58	2.08	8 (18%)
23	WO2	B	1002	-	54,116,116	64.83	8 (14%)	4,348,348	2.26	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	TAC	A	2003	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2006	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2001	22	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	D	2002	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2004	-	1/1/13/13	1/8/74/74	0/4/4/4
24	TAC	A	2005	-	1/1/13/13	1/8/74/74	0/4/4/4

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	1008	WO2	P2-OP5	475.51	8.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	1010	WO2	P2-OP5	475.51	8.56	1.52
23	A	1581	WO2	P2-OP5	475.49	8.56	1.52
23	B	1001	WO2	P2-OP5	475.48	8.56	1.52
23	G	1006	WO2	P2-OP5	475.48	8.56	1.52

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	2002	TAC	C1-C1C-C12	6.98	118.06	109.88
24	A	2003	TAC	C1-C1C-C12	6.96	118.04	109.88
24	A	2006	TAC	C1-C1C-C12	6.96	118.04	109.88
24	A	2005	TAC	C1-C1C-C12	6.94	118.02	109.88
24	A	2004	TAC	C1-C1C-C12	6.91	117.98	109.88

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	2001	TAC	C4
24	A	2003	TAC	C4
24	A	2004	TAC	C4
24	A	2005	TAC	C4
24	A	2006	TAC	C4

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	2001	TAC	C41-C4-N4-C42
24	A	2003	TAC	C41-C4-N4-C42
24	A	2004	TAC	C41-C4-N4-C42
24	A	2005	TAC	C41-C4-N4-C42
24	A	2006	TAC	C41-C4-N4-C42

There are no ring outliers.

11 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	2001	TAC	14	0
24	D	2002	TAC	12	0
23	K	1014	WO2	4	0
24	A	2004	TAC	50	0
23	G	1006	WO2	3	0

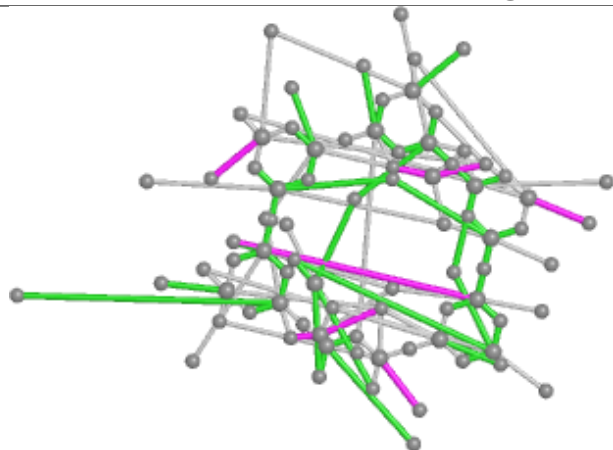
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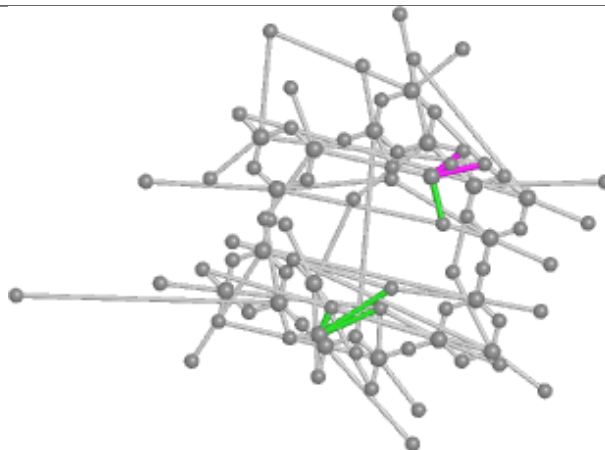
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	1001	WO2	1	0
23	E	1005	WO2	1	0
24	A	2005	TAC	42	0
23	J	1009	WO2	1	0
24	A	2003	TAC	32	0
24	A	2006	TAC	21	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

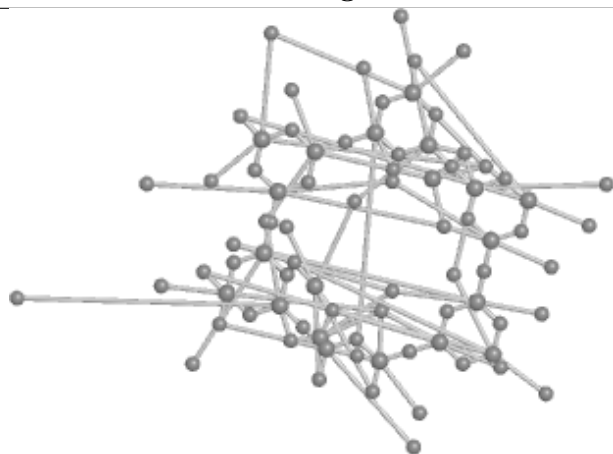
Ligand WO2 A 1582



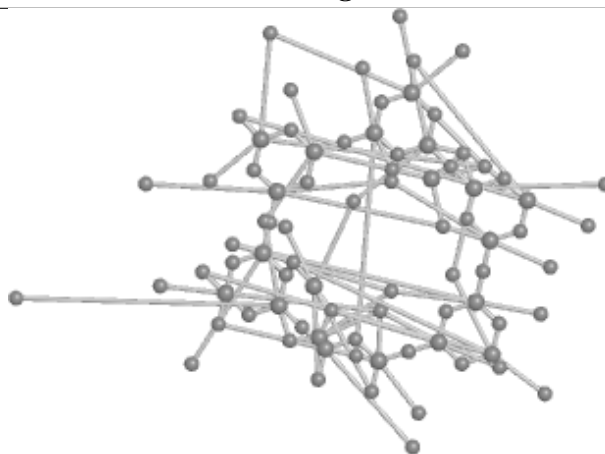
Bond lengths



Bond angles

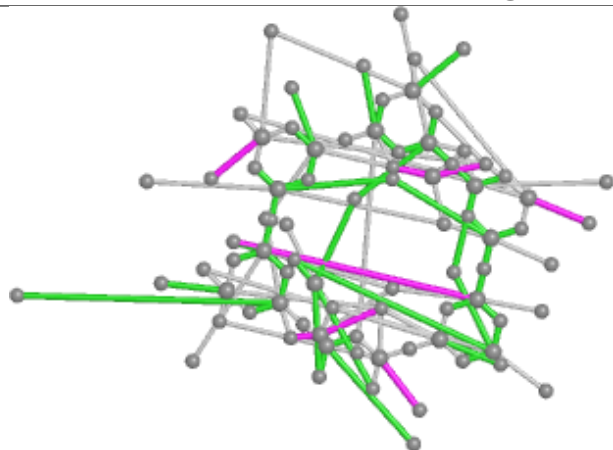


Torsions

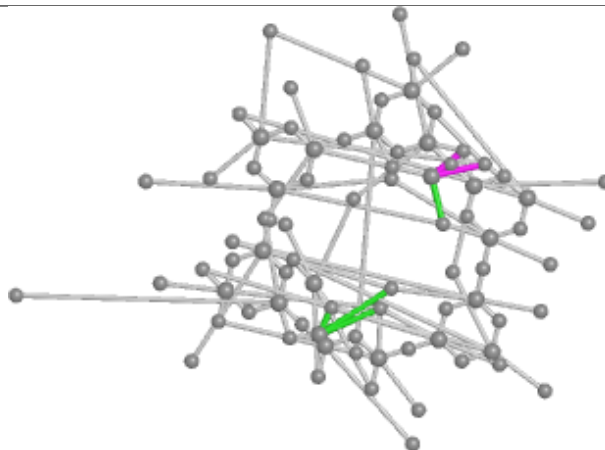


Rings

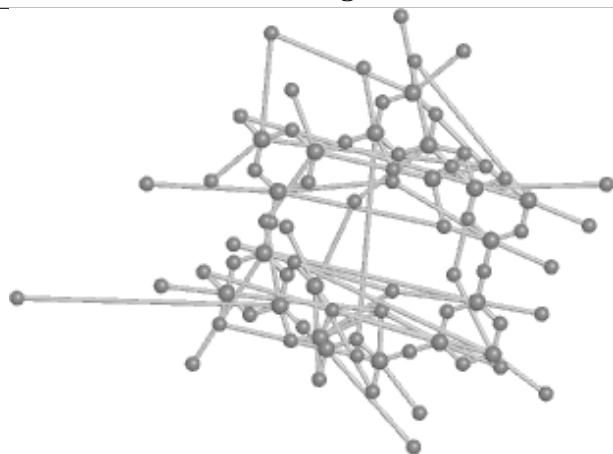
Ligand WO2 A 1579



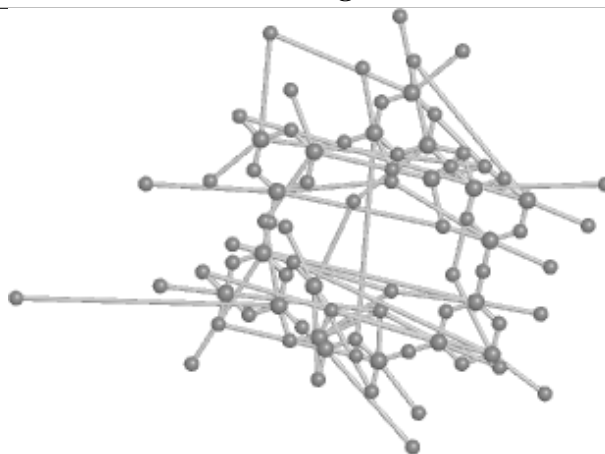
Bond lengths



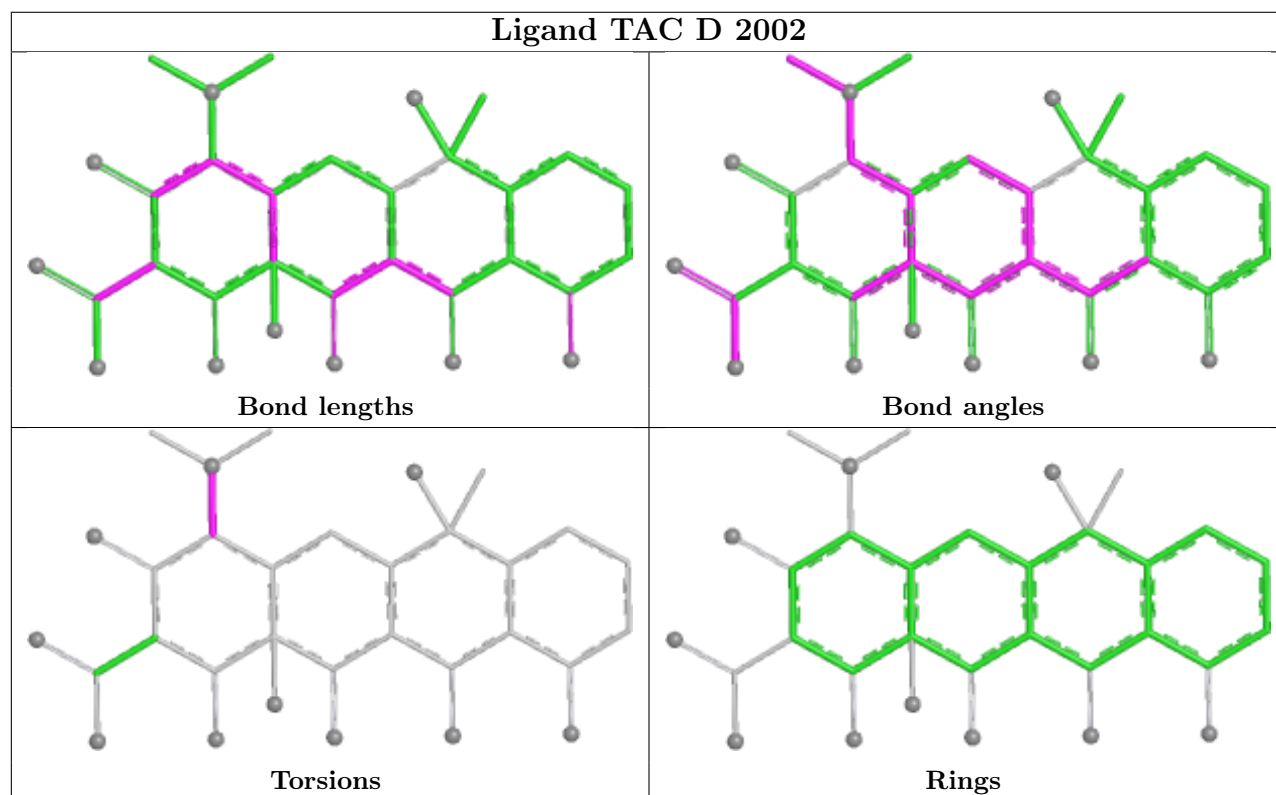
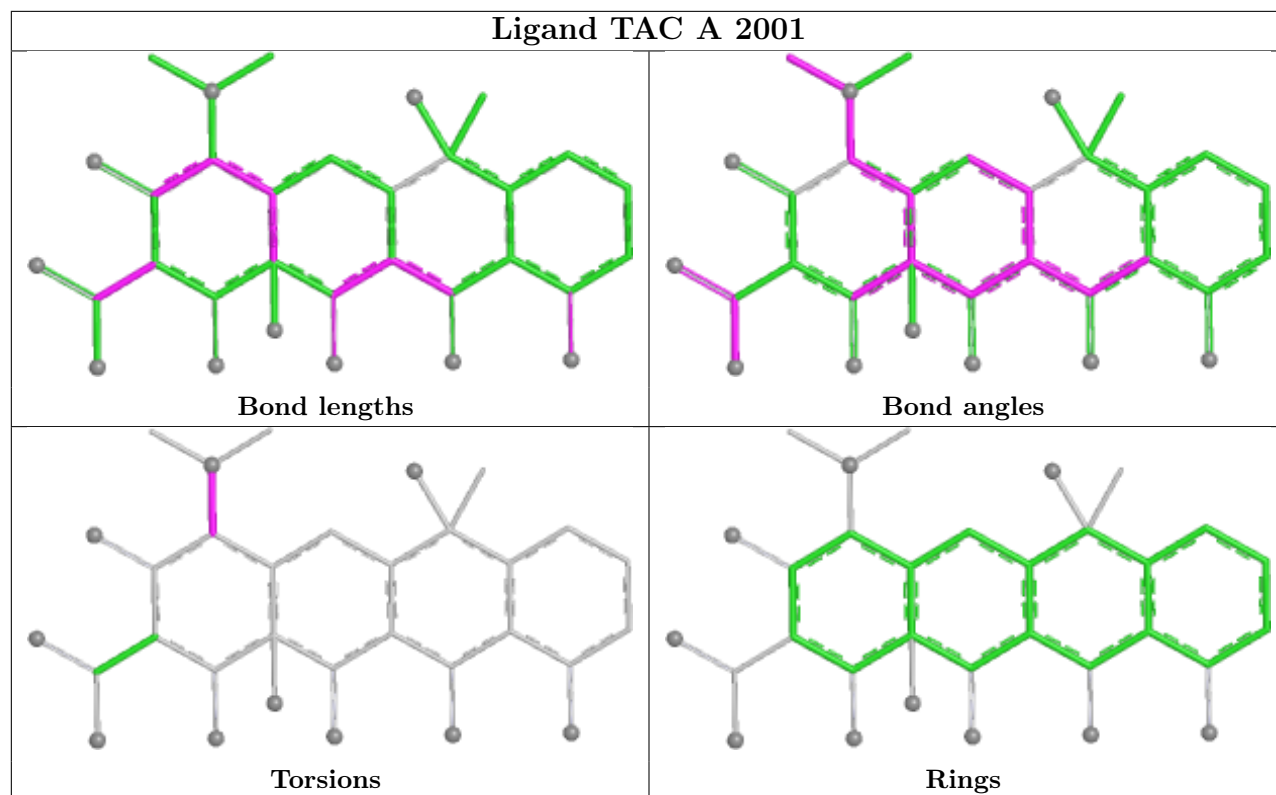
Bond angles



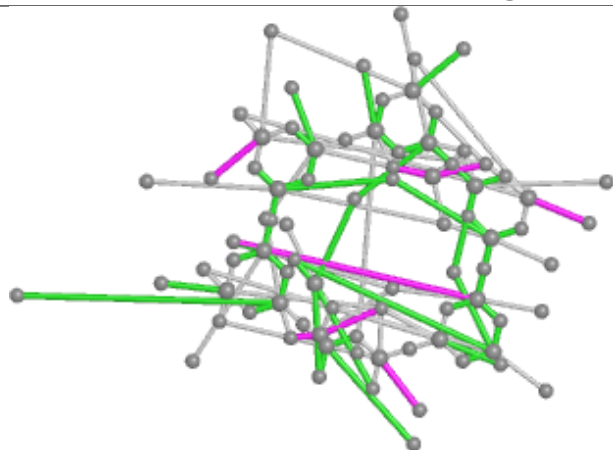
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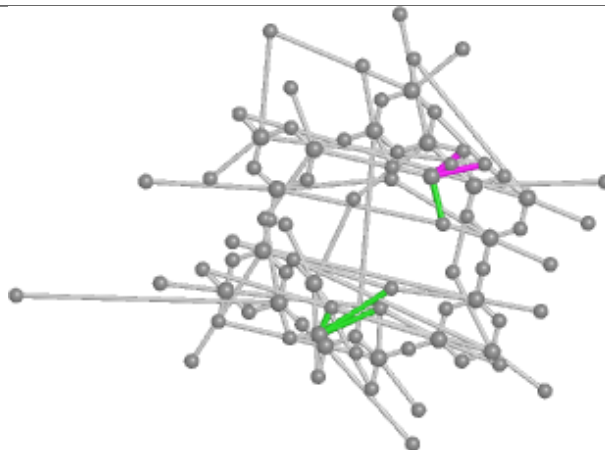
Rings



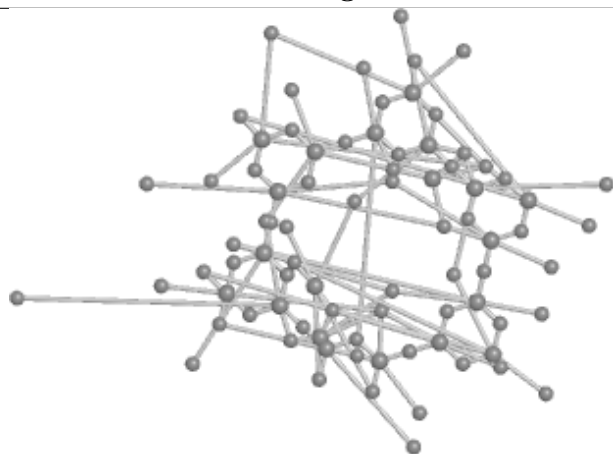
Ligand WO2 K 1014



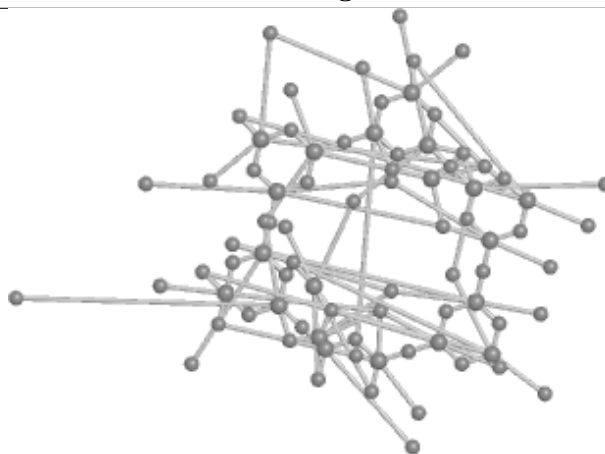
Bond lengths



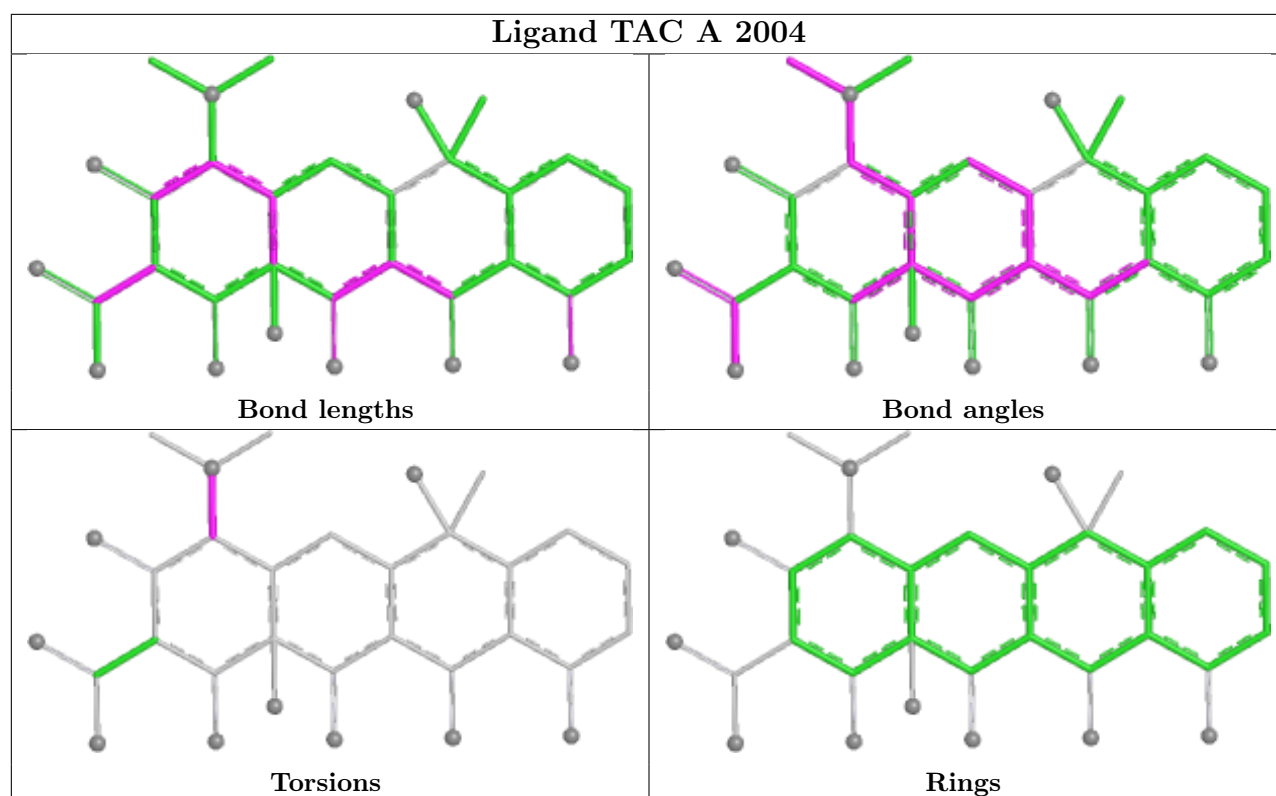
Bond angles



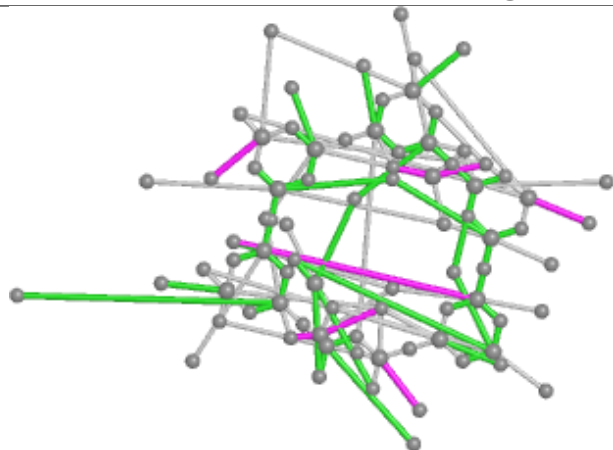
Torsions



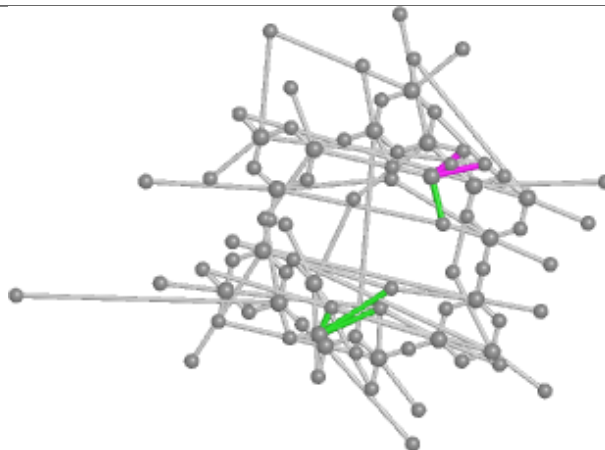
Rings



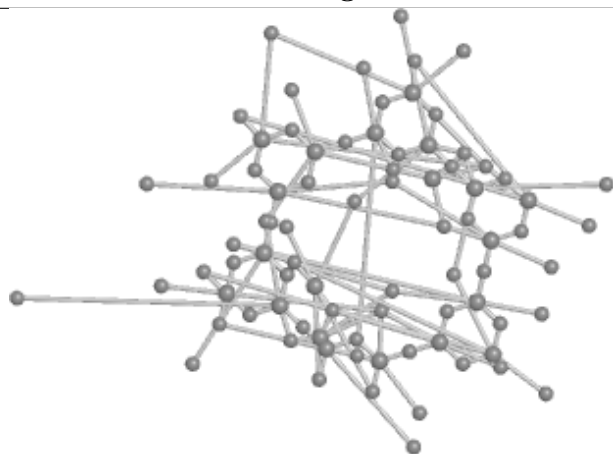
Ligand WO2 D 1012



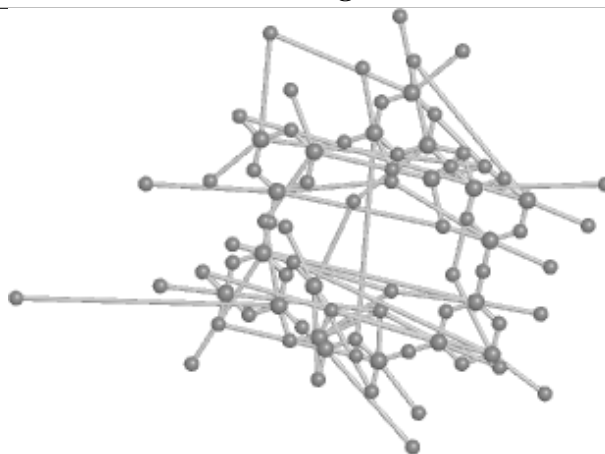
Bond lengths



Bond angles

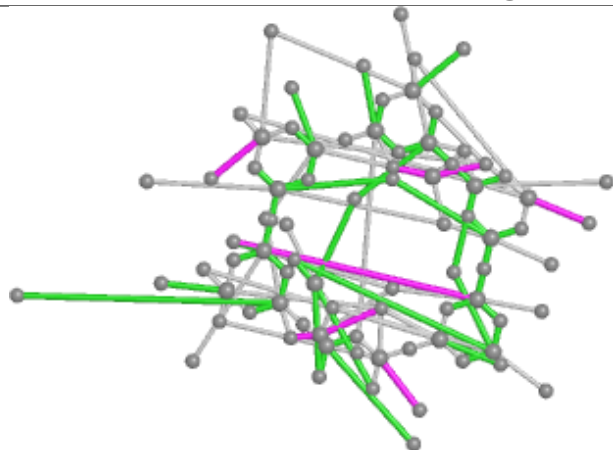


Torsions

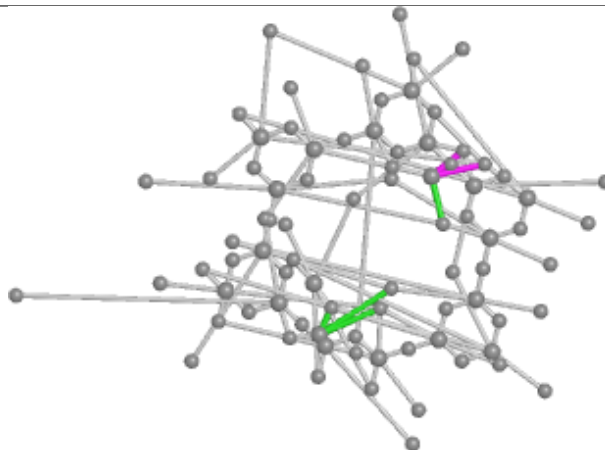


Rings

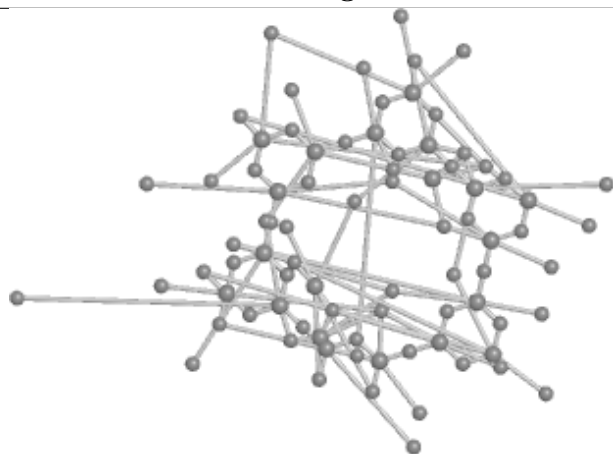
Ligand WO2 G 1006



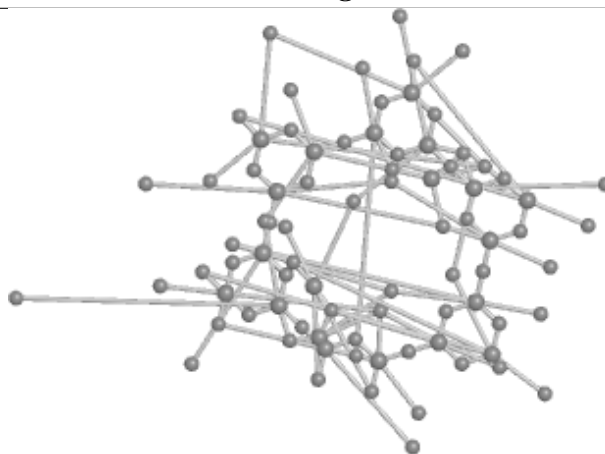
Bond lengths



Bond angles

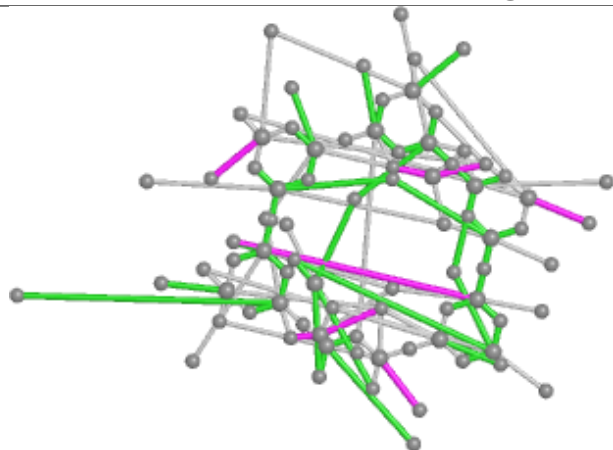


Torsions

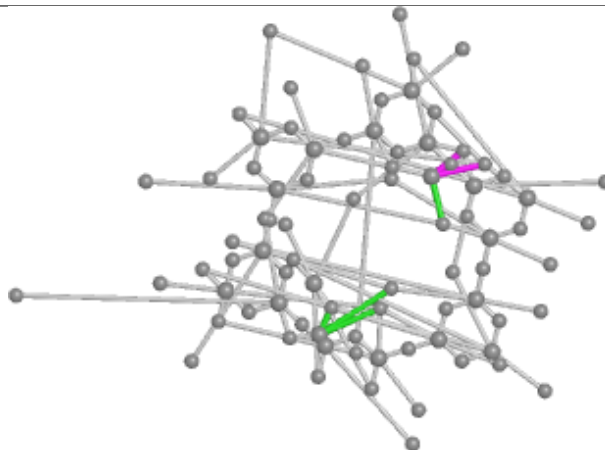


Rings

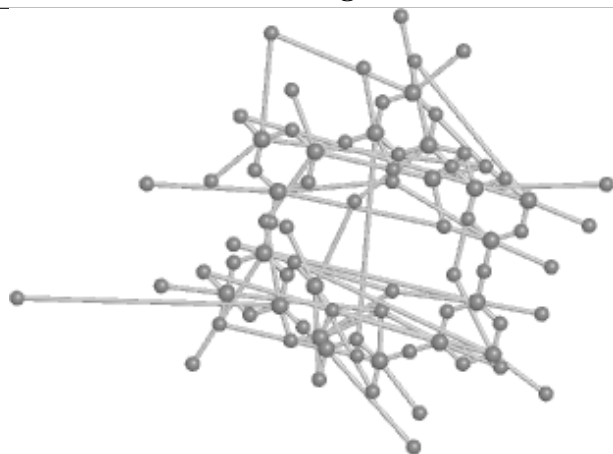
Ligand WO2 A 1581



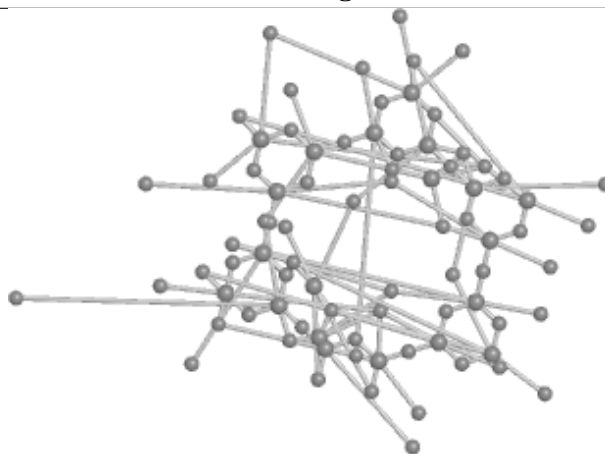
Bond lengths



Bond angles

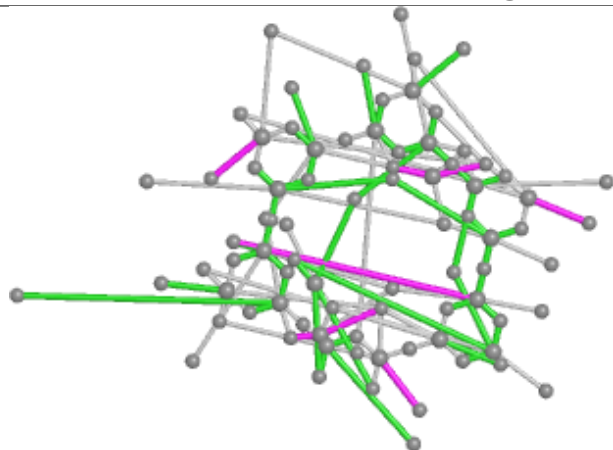


Torsions

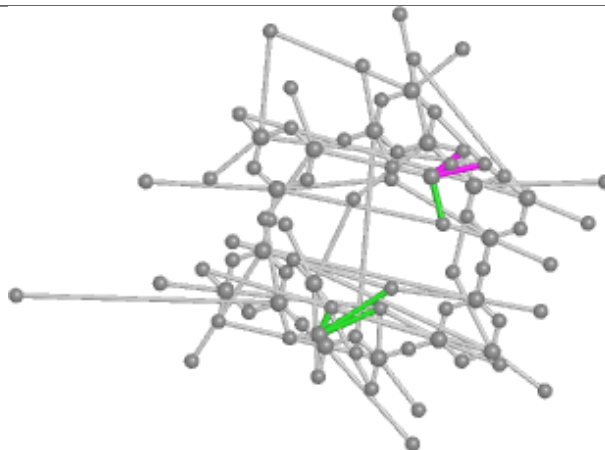


Rings

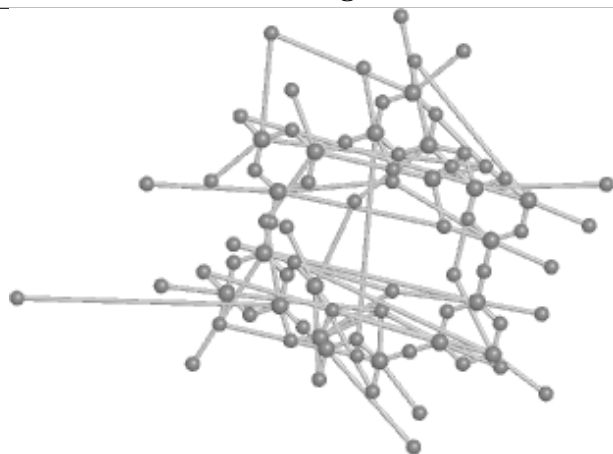
Ligand WO2 H 1010



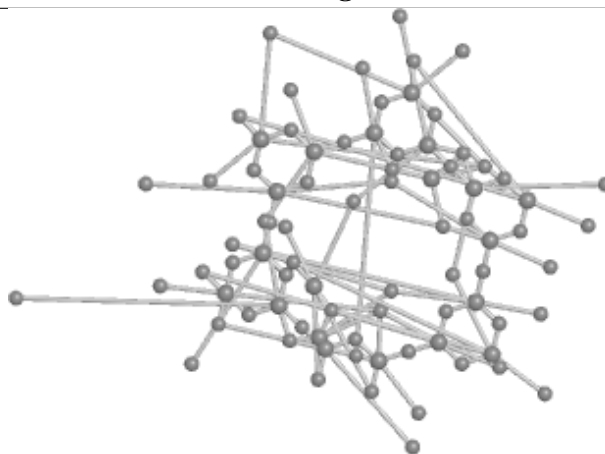
Bond lengths



Bond angles

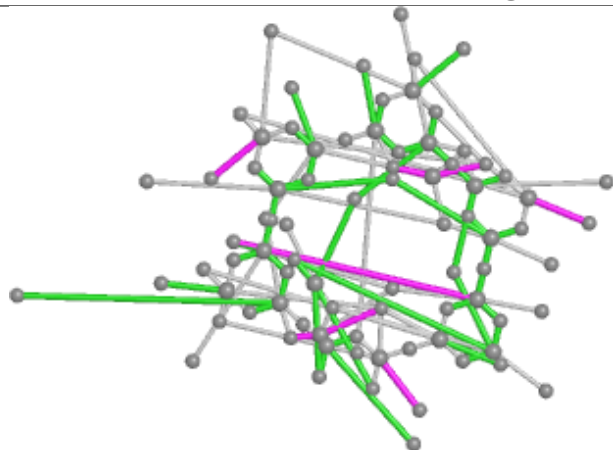


Torsions

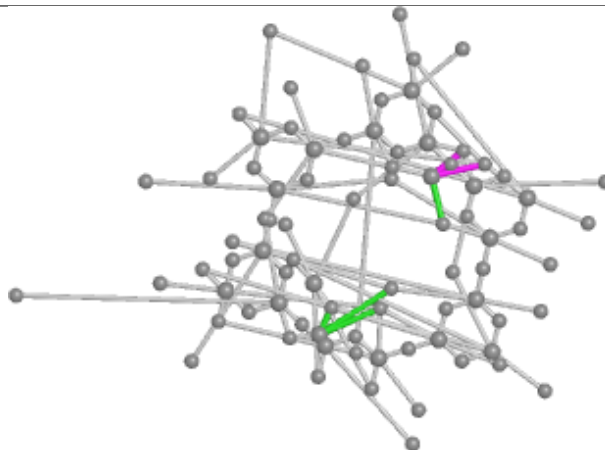


Rings

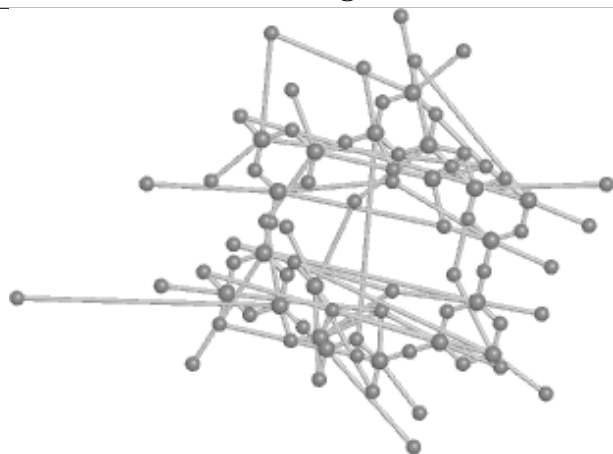
Ligand WO2 B 1001



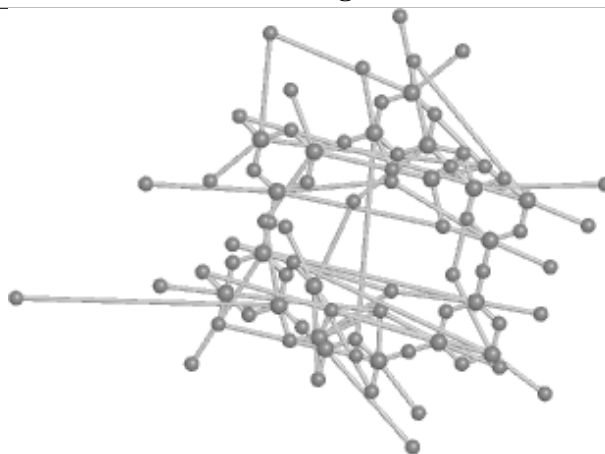
Bond lengths



Bond angles

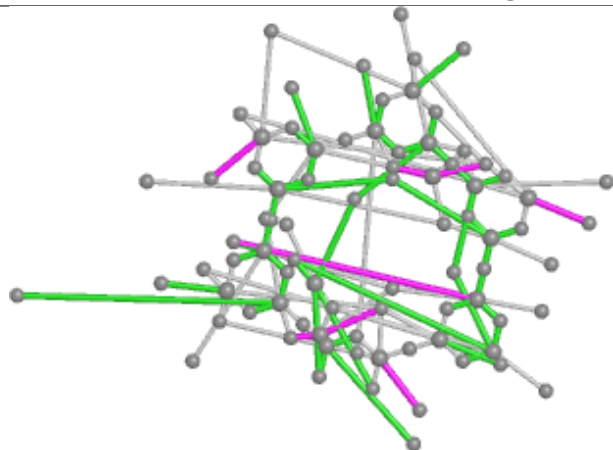


Torsions

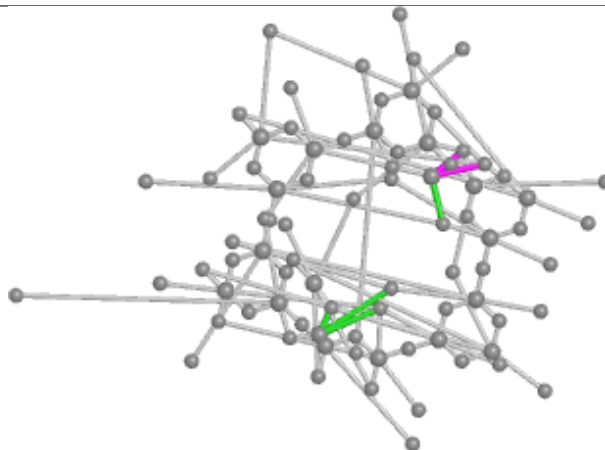


Rings

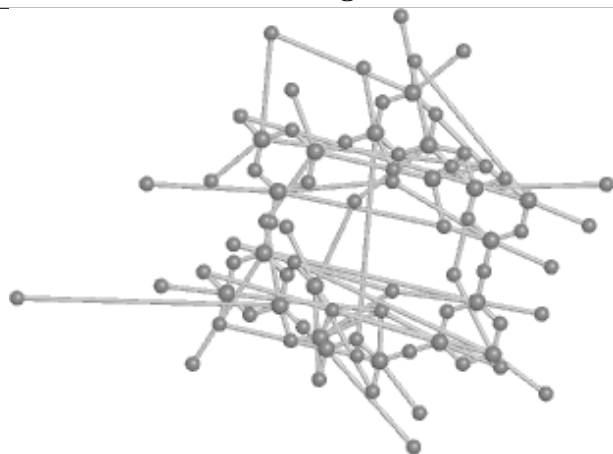
Ligand WO2 A 1580



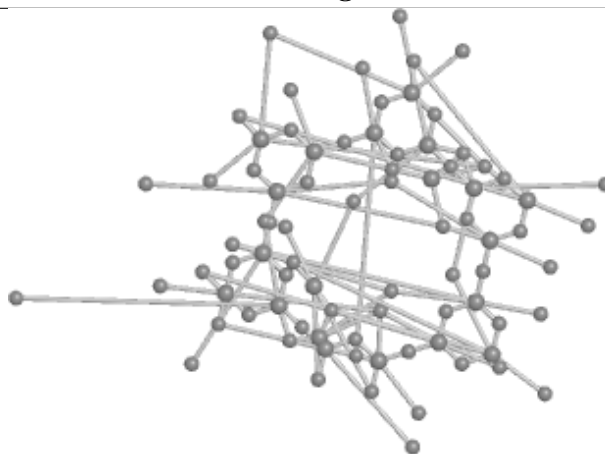
Bond lengths



Bond angles

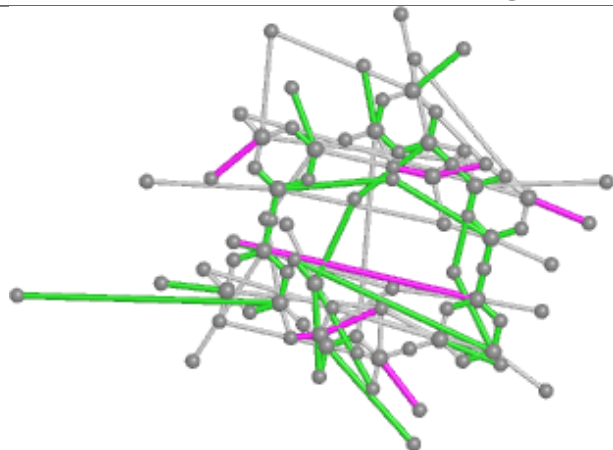


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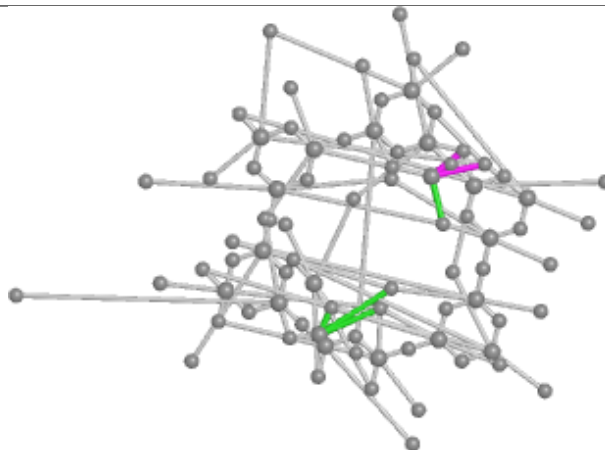


Rings

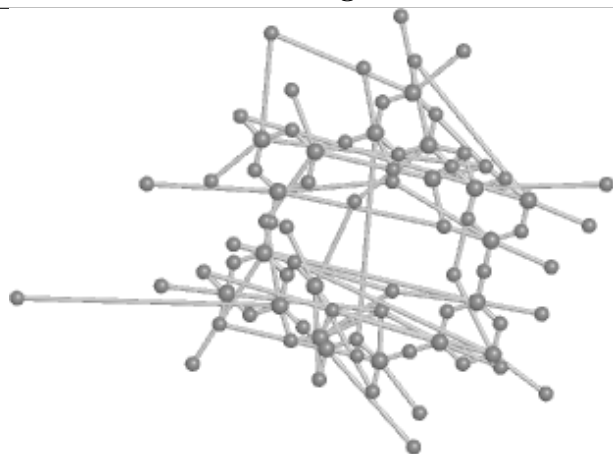
Ligand WO2 E 1005



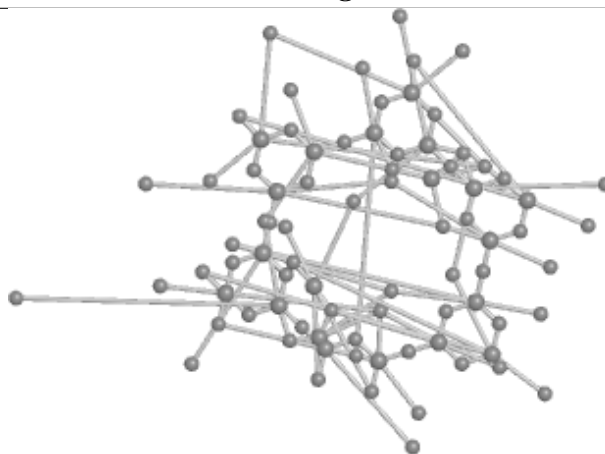
Bond lengths



Bond angles

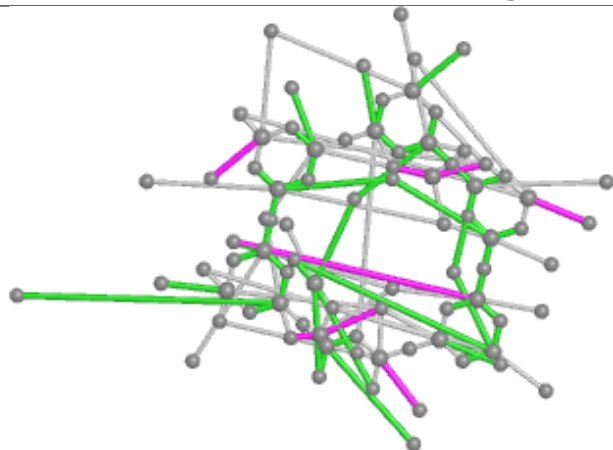


Torsions

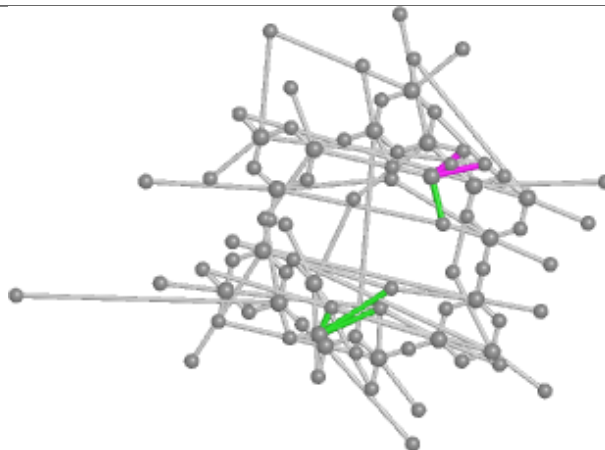


Rings

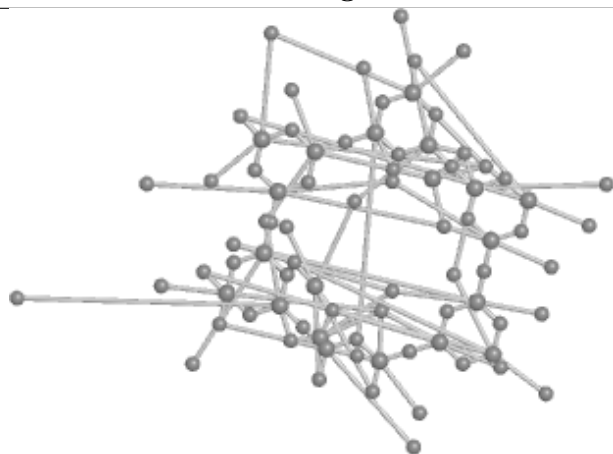
Ligand WO2 B 1004



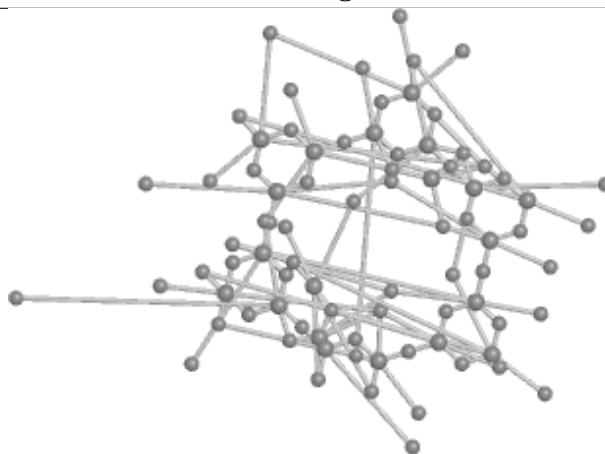
Bond lengths



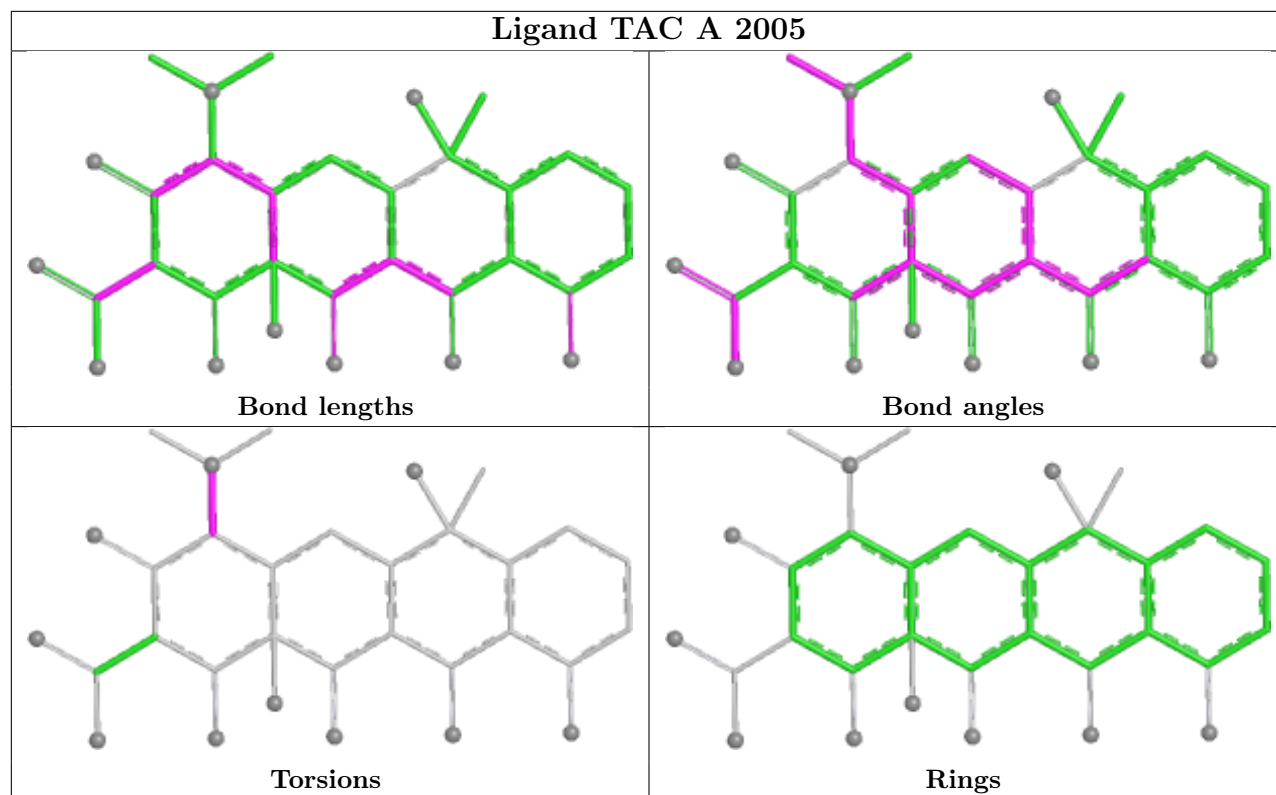
Bond angles



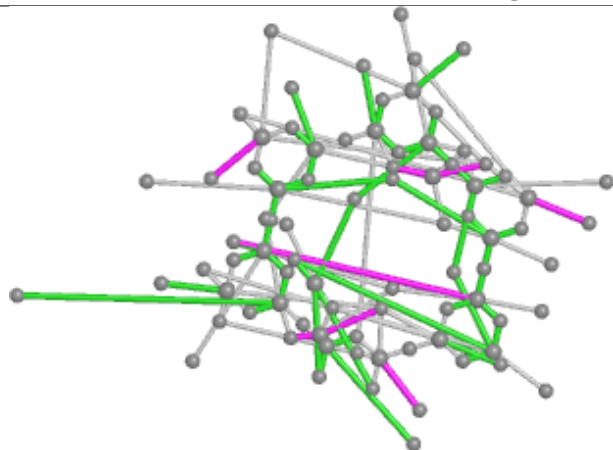
Torsions



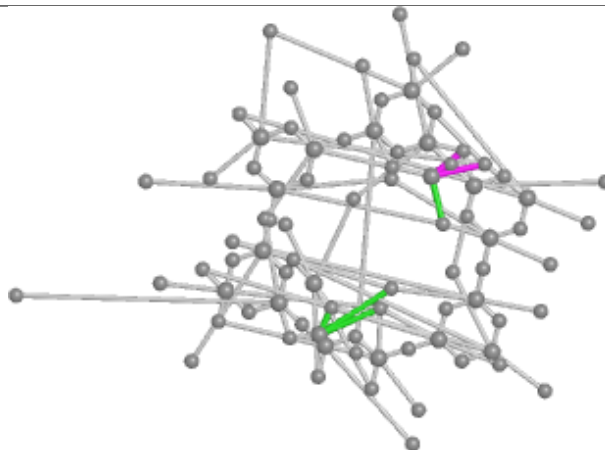
Rings



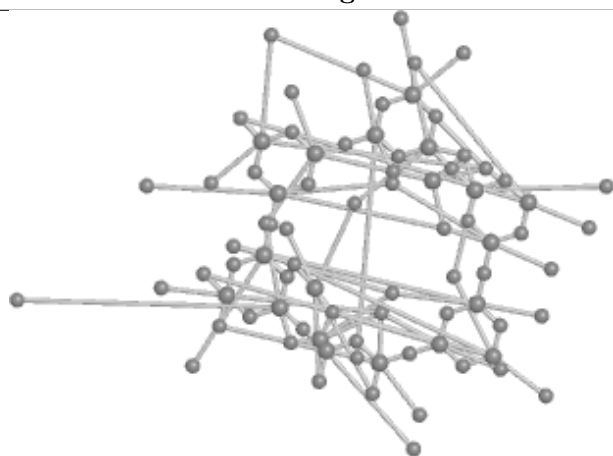
Ligand WO2 J 1009



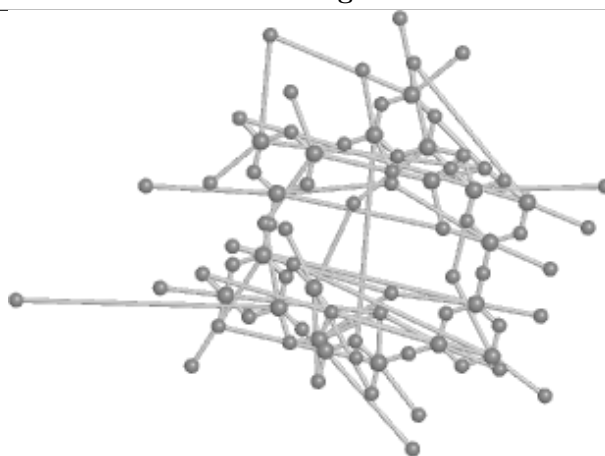
Bond lengths



Bond angles

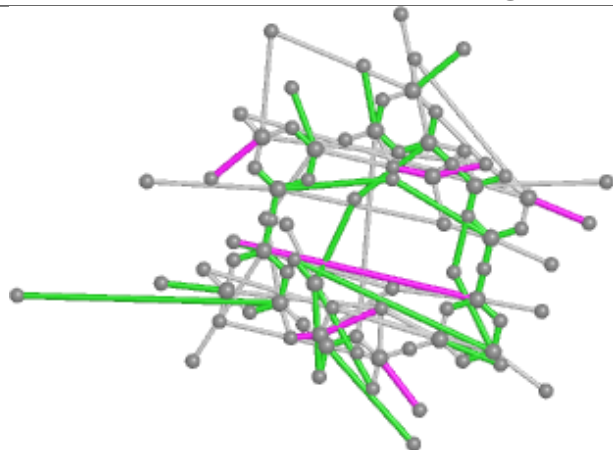


Torsions

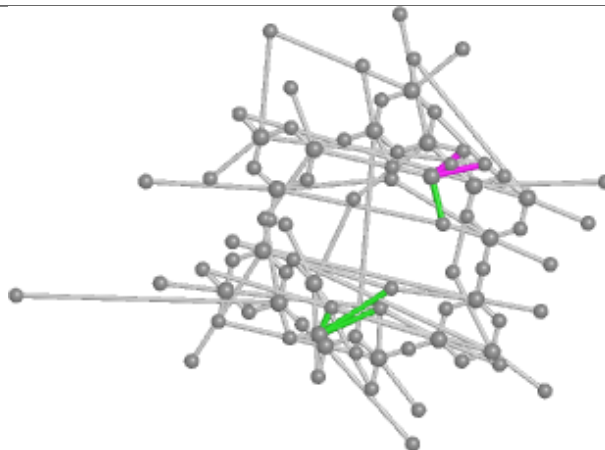


Rings

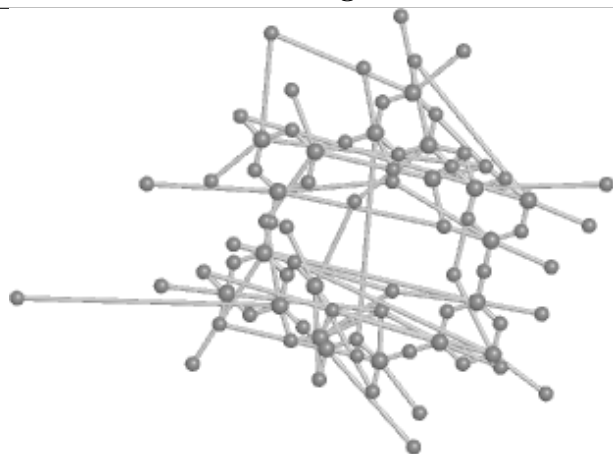
Ligand WO2 R 1008



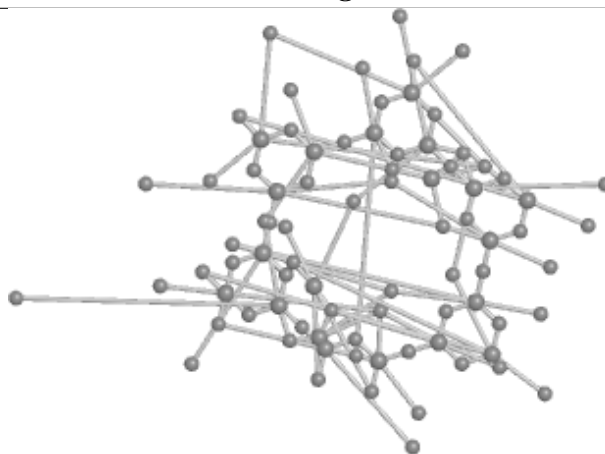
Bond lengths



Bond angles

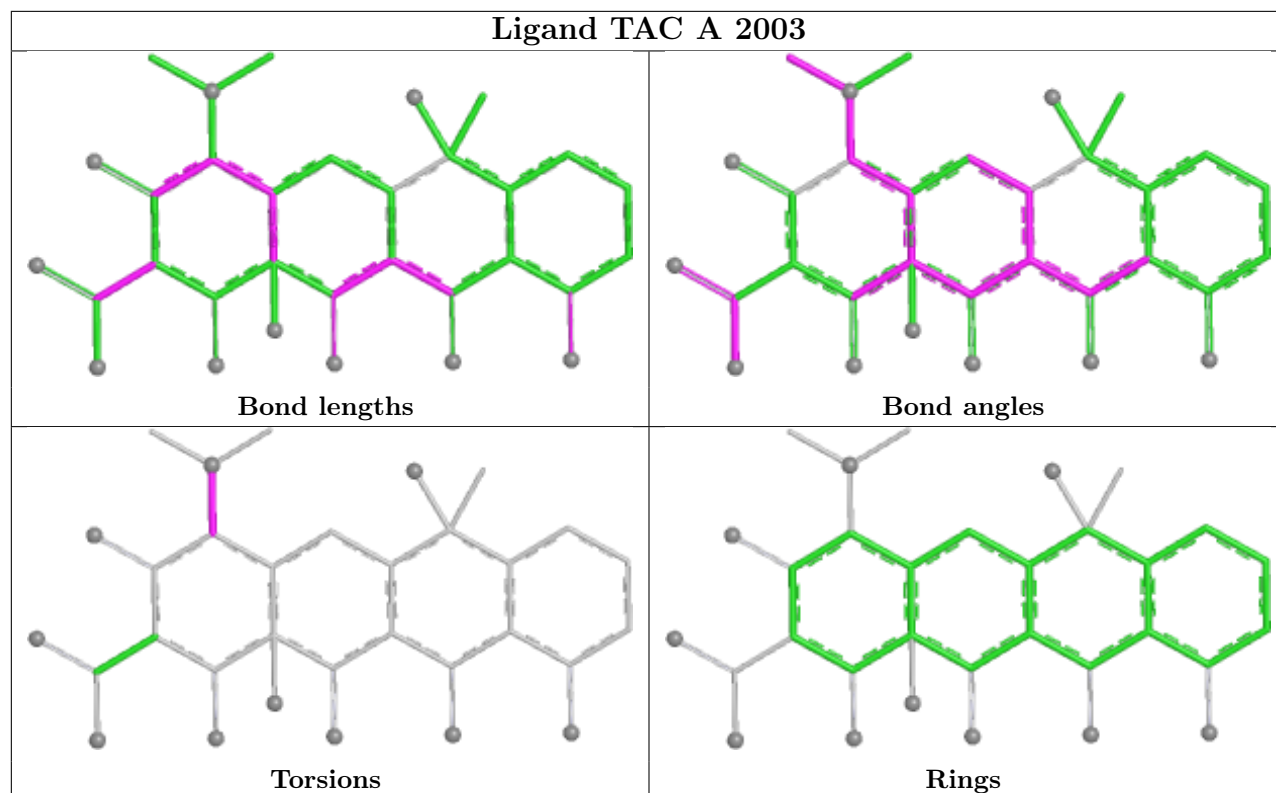


Torsions

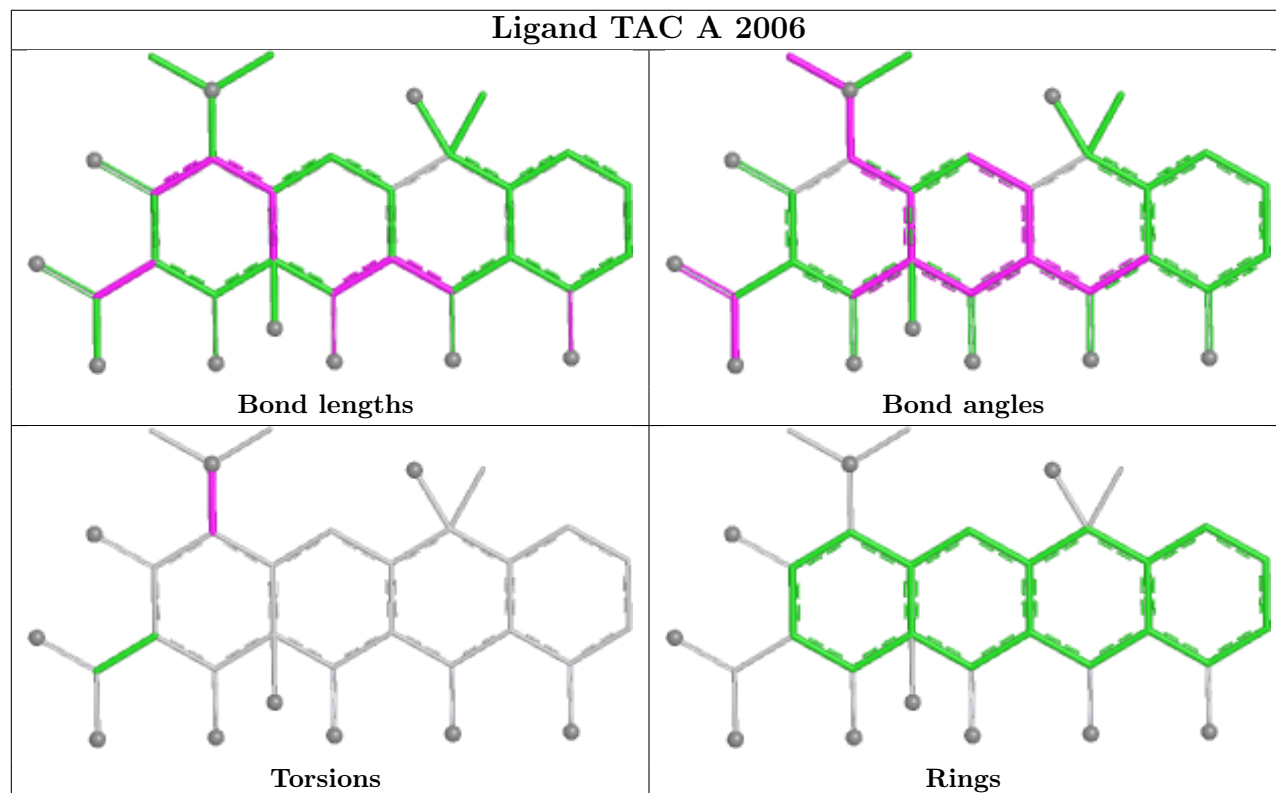


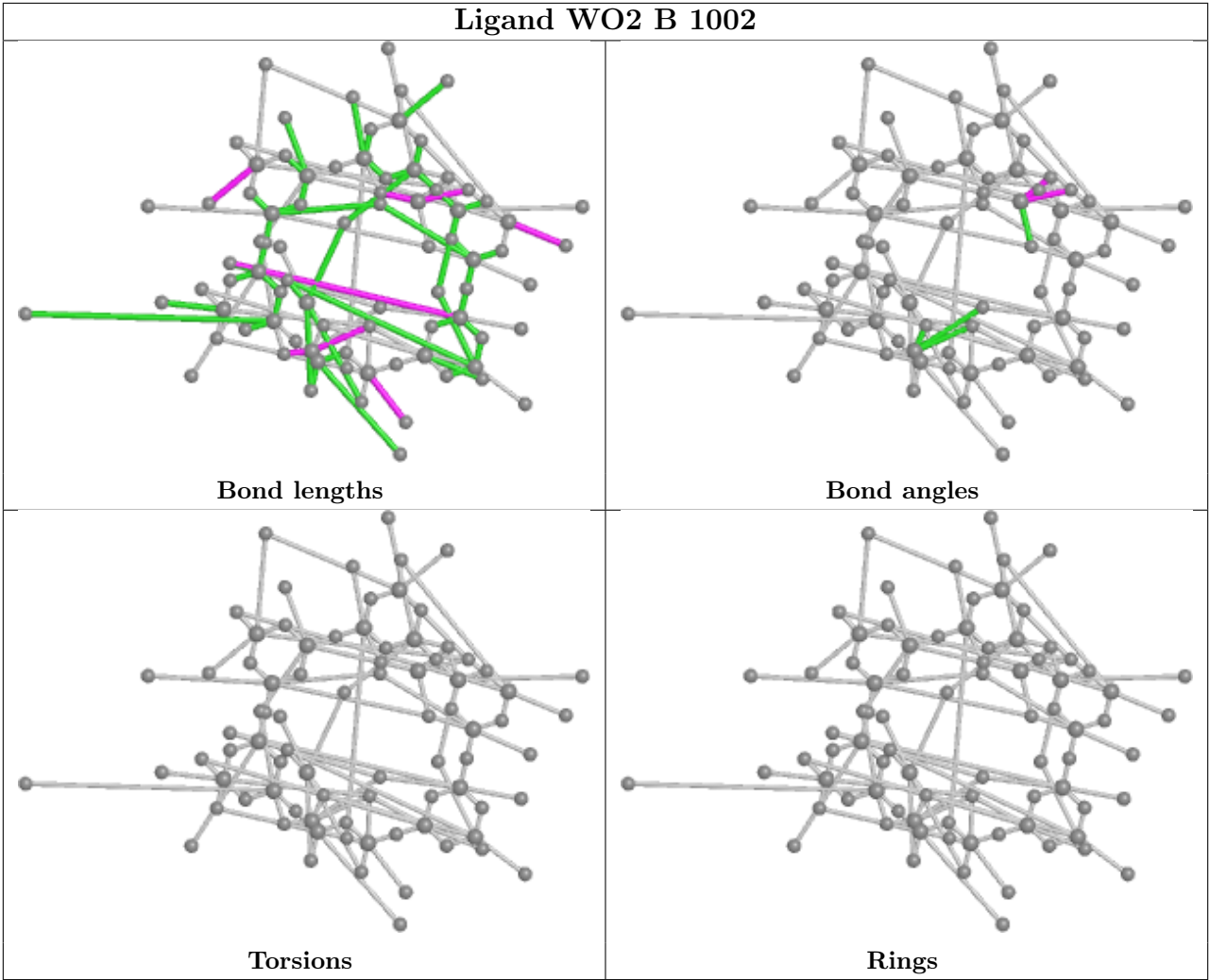
Rings

Ligand TAC A 2003



Ligand TAC A 2006





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	822:U	O3'	823:C	P	1.82

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.